Optimized perturbation theory for bound states: toy model and realistic problem.

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February 1, 2008

Abstract

Within quantum mechanics model we study the problem of resummation of an asymptotic perturbation series for bound state parameters via optimization of the perturbative expansion. A possible application of the method to the positronium lifetime calculation is also briefly considered.

PACS number(s): 11.10.Jj, 11.10.St

1 Introduction

A discrepancy between the experimental result [1] and theoretical predictions [2] for the orthopositronium width found quite a time ago still persists in spite of rigorous efforts to improve both theoretical computations and experimental data. By now an agreement on theoretical estimates for the width in the next-to-leading order is obtained and this agreed estimate is smaller than the experimental number by three standard deviations that causes some discomfort because it forces to allow quite big contribution of higher orders. The difference with experiment could be accounted for if future calculations of the order $(\alpha/\pi)^2$ coefficient determine it to be of order 250 ± 40 [1]. The anomalously large next-to-leading correction can appear accidently in a sense that in higher orders corrections become small but it can also be a signal of bad convergence of the series in fine structure constant for the positronium bound energy (width). This does not seem impossible since in most of physically interesting models of quantum field theory the conventional perturbation theory forms the asymptotic series in coupling constant that can be used for calculation of the Green's functions only if the effective parameter of the expansion is small enough. However when the exact solution is absent it is difficult to determine if the asymptotic expansion is applicable to compute some physical quantity and the value $\alpha = 1/137$ can be too large for the expansion in α being a good instrument in study of the orthopositronium width though it allows to compute another quantities, for example, the electron anomalous magnetic moment with high precision. Therefore it is instructive to try to go beyond the asymptotic expansion and improve the ordinary perturbation theory for orthopositronium width.

Some methods have been suggested to improve a convergence of the conventional perturbation theory. The basic idea of the optimized δ expansion is to introduce the artificial parameter δ which interpolates between the theory we intend to solve with Hamiltonian H, and another theory, with Hamiltonian $H_0(\lambda)$ (λ is a set of auxiliary parameters not present in the original theory), which is soluble and reflects the main properties of the theory we are interested in. One defines a new Hamiltonian depending on δ

$$H_\delta = H_0(\lambda) + \delta(H - H_0(\lambda)). \tag{1}$$

Then any desired quantity is evaluated as a perturbation series in δ, which is set equal to unity at the end of the calculations. The convergence of the series is achieved by optimization procedure [3] *i.e.* by fixing the parameters λ at every finite order of the expansion according to principle of minimal sensitivity (PMS) at the point where the result is least sensitive to their variation or principle of fastest apparent convergence (FAC) at the point where the next term in the series vanishes or somewhat else. Though above procedure is not rigorous it gives good numerical results in most of the cases. The method has been mostly advanced in studying the anharmonic oscillator [4] where the convergence has been rigorously established [5].

Thus it seems instructive to optimize the perturbation theory in analysis of the positronium bound state. However the calculation of the correction to the orthopositronium width is very involved even in the case of ordinary α expansion. Therefore it is useful to consider the simplest model that, nevertheless, retains most relevant features of the real problem and, as we hope, can help to gain some intuition to cure the difficulties with positronium.

2 The model

The problem we will study is the ground state in spectrum of the stationary Schrödinger equation in three dimensions

$$\left(-\Delta + U(\mathbf{r})\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{2}$$

where we imply $2m = \hbar = 1$ and

$$U(\mathbf{r}) = \begin{cases} -\left(\frac{\pi^2}{4} + \alpha\right) + \alpha^2 r, & r < 1, \\ 0, & r > 1. \end{cases} \tag{3}$$

At $r < 1$ the potential (3) consists of two parts: one is a constant and another depends linearly on r. The Schrödinger equation with the constant part of the potential only has bound states for any positive α with the ground state energy determined by the equation

$$\sqrt{-E_0} = \sqrt{\frac{\pi^2}{4} + \alpha}\ \cot\left(\sqrt{\frac{\pi^2}{4} + \alpha + E_0}\right). \tag{4}$$

Therefore if α is small enough we can search for the ground state energy of eq. (2) using perturbation theory and consider the constant part of the potential to be responsible for creation of the bound state while the linear term is a perturbation because it is suppressed by an extra power of α (the parameter α should not be confused with the fine structure constant).

On the other hand the exact solution of eq. (2) is known and leads to the equation for the ground state energy

$$\sqrt{-E} = \alpha^{2/3}\left(\frac{\mathrm{Bi}(\xi_0)\mathrm{Ai}'(\xi_1) - \mathrm{Ai}(\xi_0)\mathrm{Bi}'(\xi_1)}{\mathrm{Bi}(\xi_0)\mathrm{Ai}(\xi_1) - \mathrm{Ai}(\xi_0)\mathrm{Bi}(\xi_1)}\right),$$
$$\xi_0 = -\alpha^{-4/3}\left(\frac{\pi^2}{4} + \alpha + E\right), \quad \xi_1 = -\alpha^{-4/3}\left(\frac{\pi^2}{4} + \alpha - \alpha^2 + E\right) \tag{5}$$

where Ai and Bi are Airy functions [6]. Using the asymptotic expansion of Airy functions at large negative ξ_i (small α) we obtain an asymptotic series for the ground state energy

$$E(\alpha) \sim \tilde{E}(\alpha) \equiv -\frac{\alpha^2}{4}\left(1 - \left(\frac{3}{2} + \frac{2}{\pi^2}\right)\alpha + \left(\frac{21}{16} - \frac{11}{6\pi^2} + \frac{13}{\pi^4}\right)\alpha^2 - \right.$$
$$\left. - \left(\frac{39}{32} - \frac{41}{8\pi^2} + \frac{35}{6\pi^4} + \frac{26}{\pi^6}\right)\alpha^3 + \ldots\right). \tag{6}$$

Substituting numerical values for the coefficients of the expansion (6)

$$\tilde{E}(\alpha) = -\frac{\alpha^2}{4}\left(1 - 1.7026\alpha + 1.2602\alpha^2 - 0.7864\alpha^3 + \ldots\right) \tag{7}$$

we find that the series merely reveals bad convergence near the point $\alpha \sim 1$. In fact the series diverges for any positive α because the coefficients of the expansion (6) in high orders grow factorially. That reflects the presence of a singularity of the function $E(\alpha)$ at the origin of the complex α plane. The form of the singularity can be found directly

from eq. (5): $E(\alpha)$ has a cut along negative semiaxis and a branching point at $\alpha = 0$. For sufficiently small $|\alpha|$ it is an analytical function for $-\pi < \arg\alpha < \pi$ therefore the series (6) is Borel recoverable [7] *i.e.* we can extract complete information on the function $E(\alpha)$ from its asymptotic expansion. Presence of the singularity in the Green's function of eq. (2) reflects the fact that at $\alpha = 0$ the spectrum of eq. (2) changes qualitatively and a discrete part of the spectrum appears.

Such a singularity does not ultimately lead to divergence of the expansion of a bound state energy. For example, the ground state energy of the Schrödinger equation with the constant part of the potential (3) is expanded in the convergent series for any finite positive α

$$E_0(\alpha) = -\frac{\alpha^2}{4}\left(1 - \left(\frac{1}{2} - \frac{2}{\pi^2}\right)\alpha + \left(\frac{5}{16} - \frac{11}{6\pi^2} - \frac{3}{\pi^4}\right)\alpha^2 - \right.$$
$$\left. - \left(\frac{7}{32} - \frac{13}{8\pi^2} - \frac{3}{2\pi^4} - \frac{6}{\pi^6}\right)\alpha^3 + \ldots\right). \tag{8}$$

So there is no implicit singularity in the series for $E_0(\alpha)$. However after inclusion of the perturbation such a singularity appears and the full series (6) becomes divergent. This, in a sense, simulates the positronium bound state where the non-relativistic Coulomb potential that is taken to build the leading order bound state Green's function does not lead to implicit singularity of bound state energy in the fine structure constant while the relativistic corrections result, as we suppose, in the divergent series. Thus we can use our quantum mechanics analog as a test model for further analysis of the positronium.

3 Optimized expansion

Our purpose now is to develop the optimized perturbation theory (OPT) for our toy model. Following the general idea we have to choose the form of the "unperturbed" Hamiltonian. The Hamiltonian

$$H_0(\alpha') = -\Delta + U_0(\alpha',\ \mathbf{r}) \tag{9}$$

where

$$U_0(\alpha',\ \mathbf{r}) = \begin{cases} -\left(\frac{\pi^2}{4}+\alpha'\right), & r<1, \\ 0, & r>1, \end{cases} \tag{10}$$

is the potential of the spherical well with changeable depth seems to be the most appropriate choice. Here the set of parameters λ in eq. (1) is reduced to the single parameter α' characterizing the depth of the well. The ordinary perturbation theory corresponds to $\alpha' = \alpha$ and $\delta = 1$. Making the expansion in δ and setting $\delta = 1$ we obtain in n-th order the series for the ground state energy

$$\begin{aligned} E_n(\alpha,\alpha') &= E^{(0)}(\alpha') + E^{(1)}(\alpha,\alpha') + \ldots + E^{(n)}(\alpha,\alpha'), \\ E^{(0)}(\alpha') &= -\frac{\alpha'^2}{4}\left(1-\left(\frac{1}{2}-\frac{2}{\pi^2}\right)\alpha' + \left(\frac{5}{16}-\frac{11}{6\pi^2}-\frac{3}{\pi^4}\right)\alpha'^2+\ldots\right), \\ E^{(1)}(\alpha,\alpha') &= \frac{(\alpha'-\alpha)\alpha'}{2}\left(1-\left(\frac{3}{4}-\frac{3}{\pi^2}\right)\alpha'+\ldots\right) + \\ &+\frac{\alpha^2\alpha'}{4}\left(1+\frac{4}{\pi^2}-\left(\frac{3}{4}-\frac{2}{\pi^2}+\frac{12}{\pi^4}\right)\alpha'+\ldots\right), \\ E^{(2)}(\alpha,\alpha') &= \left(\frac{(\alpha'-\alpha)}{2}+\alpha^2\left(\frac{1}{4}+\frac{1}{\pi^2}\right)\right)^2+\ldots. \end{aligned} \tag{11}$$

where the explicit expressions for $E^{(i)}$ are expanded in α' and α. In general if $\alpha'-\alpha = O(\alpha^2)$ the effective parameter of the expansion is proportional to

$$\frac{\langle 0|U(\alpha)-U_0(\alpha')|0\rangle}{E_0(\alpha')} \sim \alpha. \tag{12}$$

So $E_n(\alpha,\alpha')$ after expansion in α correctly reproduces the first n terms of eq. (6). Thus if we are interested in only the asymptotic expansion the choice of the start approximation does not play a crucial role. If, however, we intend to go beyond the asymptotic expansion we have to choose the "unperturbed" Hamiltonian to provide the best convergence of the expansion. The most transparent and conventional way to optimize the expansion (11) is to fix the parameter α' in n-th order according to PMS (FAC) at the value α_n^{PMS} (α_n^{FAC}) so that

$$\left.\frac{\partial E_n}{\partial \alpha'}\right|_{\alpha'=\alpha_n^{PMS}} = 0, \tag{13}$$

or

$$E^{(n+1)}|_{\alpha'=\alpha_n^{FAC}} = 0. \tag{14}$$

At $n = 1$ we have

$$\alpha_1^{PMS} = \alpha\left(1 - \left(\frac{1}{2} + \frac{2}{\pi^2}\right)\alpha + \ldots\right), \tag{15}$$

$$\alpha_1^{FAC} = \alpha\left(1 - \left(\frac{1}{2} + \frac{2}{\pi^2}\right)\alpha + \ldots\right). \tag{16}$$

Since $\alpha^{\#} - \alpha = O(\alpha^2)$ where # stands for PMS or FAC we have $E^{(n)}(\alpha, \alpha^{\#}) = O(\alpha^n E^{(0)}(\alpha))$. Therefore expanding eq. (13, 14) in α we obtain at $n \to \infty$ the formal series

$$\alpha_n^{\#} \to \alpha^{\#} = \alpha(1 + a_1^{\#}\alpha + a_2^{\#}\alpha^2 + \ldots), \tag{17}$$

moreover

$$E_n(\alpha, \alpha_n^{FAC})|_{n\to\infty} \to E_0(\alpha^{FAC}(\alpha)). \tag{18}$$

Now we show that one can choose $\alpha^{PMS} = \alpha^{FAC}$. Let us suppose that $a_i^{PMS} = a_i^{FAC}$ for $i \leq n$. The PMS condition to determine a_{n+1}^{PMS} reads

$$\frac{\partial E_{n+1}}{\partial \alpha'}\Big|_{\alpha'-\alpha^{PMS}=O(\alpha^{n+3})} = O(\alpha^{n+1}E_0(\alpha)). \tag{19}$$

On the other hand

$$E^{(n+1)}|_{\alpha'-\alpha^{PMS}=O(\alpha^{n+2})} = O(\alpha^{n+2}E_0(\alpha)),$$

$$\tilde{E}(\alpha) - E_{n+1}|_{\alpha'-\alpha^{PMS}=O(\alpha^{n+2})} = O(\alpha^{n+2}E_0(\alpha)) \tag{20}$$

because $a_i^{PMS} = a_i^{FAC}$ for $i \leq n$. Therefore

$$\frac{\partial E_{n+1}}{\partial \alpha'}\Big|_{\alpha'-\alpha^{PMS}=O(\alpha^{n+3})} = \frac{\partial(E_{n+1} - \tilde{E}(\alpha))}{\partial \alpha'}\Big|_{\alpha'-\alpha^{PMS}=O(\alpha^{n+3})} =$$

$$= \frac{\partial(E_{n+1}|_{\alpha'-\alpha^{PMS}=O(\alpha^{n+2})} - \tilde{E}(\alpha))}{\partial\alpha'} + O(\alpha^{n+1}E_0(\alpha)) = O(\alpha^{n+1}E_0(\alpha)) \qquad (21)$$

where taking a derivative of the asymptotic series is justified because $\tilde{E}(\alpha)$ is a power series and all non-analytical in α' terms in E_{n+1} must be cancelled in higher orders and, therefore, can be omitted before taking a derivative. So condition (19) is satisfied for arbitrary a_{n+1}^{PMS} and we can put $a_{n+1}^{PMS} = a_{n+1}^{FAC}$. Since $a_i^{PMS} = a_i^{FAC}$ for $i = 1$ (see eqs. (15, 16)) one can choose $a_i^{PMS} = a_i^{FAC}$ for any i whence $\alpha^{PMS} = \alpha^{FAC}$.

Thus in the limit $n \to \infty$ all corrections in the optimized expansion (11) vanish both for PMS and FAC optimization prescription and we obtain

$$E_n(\alpha, \alpha_n^{\#}) \to E_0(\alpha^{\#}(\alpha)) = E(\alpha). \qquad (22)$$

Since the function $E_0(\alpha^{\#})$ can be expanded in the convergent series in $\alpha^{\#}$ (eq. (8)) the singularity of the function $E(\alpha)$ at $\alpha = 0$ is absorbed by the function $\alpha^{\#}(\alpha)$ *i.e.* the series (16) is a divergent asymptotic expansion. However we can search for the values $\alpha_n^{\#}$ which satisfy eqs. (13, 14) at every order numerically rather than as a series in α. In Fig. 1 and Fig. 2 we plot the functions $E_1(1.0, \alpha')$ and $E^{(1)}(1, \alpha')/E^{(0)}(1, \alpha')$ to show a typical pictures that are used to determine $\alpha^{\#}$. Thus for $\alpha = 1.0$ we obtain $\alpha_1^{PMS} = 0.310$ and $\alpha_0^{FAC} = 0.304$.

Thus we have three kinds of perturbative expansion: the asymptotic series, the standard perturbation theory and OPT. The asymptotic series seems to be the most primitive tool and we expect to obtain the best results using OPT. This assumption is completely confirmed by numerical analysis given in the next section.

4 Numerical evaluation

The results of numerical analysis are given in Tabs. $1 - 3$[1]. In Tab. 1 we establish the exact value $E(\alpha)$ along with the results of the asymptotic expansion $\tilde{E}_n(\alpha)$ up to the n-th order ($n = 0,\ 1,\ 2,\ 3$). In Tab. 2 we compare the exact value $E(\alpha)$, the result of the

[1]For the exact value and approximations of the bound energy in Tabs. $1 - 3$ the factor (-10^{-2}) is implied

optimized expansion $E_1(\alpha, \alpha_1^{PMS})$ and the results of the odinary perturbation theory up to the n-th order ($n = 0,\ 1$) *i.e.* not expanded values of $E_0(\alpha)$ and $E_1(\alpha, \alpha)$. All the $[i, j]$ Padé approximants $E^{[i,j]}(\alpha)$ with $i + j \leq 3$ are in Tab. 3.

We give numerical estimates for three different values of the parameter α that represent typical cases

1. $\alpha = 0.1$: the asymptotic expansion is applicable and justified;

2. $\alpha = 0.5$: the asymptotic expansion is applicable but one has to deal with the high orders corrections to achieve a satisfactory accuracy. An improvement of the perturbation theory is desirable;

3. $\alpha = 1.0$: the asymptotic expansion in principle can provides only $\sim 2\%$ accuracy after summation of ~ 13 terms. Then the terms start to grow. The perturbation theory must be reformulated.

As we can see a naive attempt to improve the convergence of the perturbative expansion simply keeping the exact (not expanded) value of $E_n(\alpha, \alpha)$ that sums up some next-to-leading corrections gives a good result but is essentially insufficient if α is large enough. This shows that optimization is important for convergence. Though we cannot directly demonstrate that without the optimization the series (11) becomes divergent as it takes place in the case of anharmonic oscillator [5] the numerical analysis clearly shows an advantage of optimized expansion. Indeed in all these cases the best convergence is achieved within OPT. Even for $\alpha = 1.0$ taking only the first order correction we reach $\sim 2\%$ accuracy. Using the PMS prescription we can also correctly estimate an error of the result. For example for $\alpha = 1.0$ the naive estimate is $(E^{(1)}(1.0, \alpha^{PMS})/E^{(0)}(1.0, \alpha^{PMS}))^2 \sim 0.02$ that coincides with the real uncertainty (see Tab. 1).

We should note that in all the cases the terms of α expansion taken into account in our numerical analysis are far from the critical point where the series begins to diverge. The bad convergence of the series reveals only in the fact that they decrease quite slow. On the other hand even the third order correction is hardly available within ordinary perturbation theory. So the accuracy of the perturbation theory is restricted rather by technical reasons than by asymptotic character of the series. Thus the optimization is not

only a resummation prescription that is useful in high orders of asymptotic expansion but also gives an opportunity to improve accuracy of perturbation theory in low orders. This is an important benefit especially for non-trivial systems where high orders calculations are impossible.

A remark about Padé approach is in order. As we can see some Padé approximants are closer to the exact result than the plain asymptotic expansion. However it is not possible to make a choice between various approximants until the exact result or the general structure of the series are known. Moreover in high orders where the asymptotic character of the series reveals the Padé theory becomes useless. The matter is that Padé approximants because of their specific structure can correctly reproduce only pole-like singularity while the function $E(\alpha)$ has a branching point at $\alpha = 0$.

5 The positronium bound state

The theoretical predictions for the orthopositronium width reads [2]

$$\Gamma_{o-Ps} = m\alpha^6 \frac{(2\pi^2 - 18)}{9\pi} \left[1 - 10.282 \left(\frac{\alpha}{\pi}\right) + \right.$$
$$\left. + \frac{1}{3}\alpha^2 \ln \alpha + B \left(\frac{\alpha}{\pi}\right)^2 + \ldots \right]. \qquad (23)$$

where the coefficient B has not yet been computed but it is expected to be about 250 to bring theory and experiment into agreement. The coefficients of eq. (23) tend to grow rapidly. In spite of the value $\alpha = 1/137$ seems to be small enough the contribution of the second order term is about 0.2% of the leading one. This resembles the behavior of the asymptotic series in our toy model with $0.1 < \alpha < 0.5$ where the asymptotic expansion can, in principle, provide a sufficient accuracy but it requires to compute high order terms that is not possible by pure technical reasons. So we hope that after optimization of the expansion an agreement between experimental and theoretical values will be reached already in the first order of OPT.

The main problem of OPT is to find an appropriate form of "unperturbed" action which, on the one hand reflects the main properties of the exact theory and, on the other

hand does not lead to extremely cumbersome calculations. The most direct way for the positronium bound state is as follows. By now there are two general methods to develop the systematic perturbation theory for the positronium: the non-relativistic $1/c$ expansion [8] and the method based on Bethe-Salpeter equation [9]. The non-relativistic Coulomb solution and Barbieri-Remiddi solution [10] which are used to built the leading order approximations for the positronium bound state Green's function within these approaches involve the physical fine structure constant as a parameter. In analogy with our toy model one can replace it with a changeable parameter α'. Then in every order of the new perturbation theory one has to keep the exact dependence on α' and fix it using some optimization prescription. We should emphasize that the optimized value has no direct relation to the physical fine structure constant. This is an auxiliary parameter and constructing the OPT, for example, for orthopositronium bound energy we would obtain a different value of this parameter. Unlike the case of the asymptotic α expansion two above start approximations can lead to the different results if one is interested in the optimized expansion but it is not obvious which is preferable. Though the detail analysis of the positronium is a non-trivial technical problem that is a subject of a separate publication.

To conclude we should note that an attempt to improve the perturbation theory in orthopositronium width analysis using Padé approximants has been made in ref. [11]. However it looks artificially because an information about structure of the asymptotic expansion (23) is absent. On the other hand OPT seems to be the most appropriate tool to deal with such a problem because it speeds up the convergence of the perturbation series choosing the most natural start approximation for a *specific* model not by an extraneous mathematical trick. This is an automatic summation device that need not an input information on the form of the singularity of the bound state Green's function in the coupling constant but reproduce it via optimization. This feature can be merely observed in our toy model where the form of the singularity of the ground state energy at $\alpha = 0$ in the auxiliary and original theories are essentially different but OPT reproduces the correct singular α dependence that is absorbed by the optimized value of auxiliary parameter α'. This general property of optimized perturbation theory allows to cope even with Borel

non-summable series [5] while a class of the problems where the Padé theory can be successfully applied is quite restricted.

Acknowledgments

This work is supported in part by Russian Fund for Fundamental Research under Contract No. 93-02-14428 and by Soros Foundation. The work of A.A.Penin has been made possible by a fellowship of Royal Swedish Academy of Sciences and is carried out under the research program of International Center for Fundamental Physics in Moscow.

Figure Captions

Fig. 1. The curve line depicts the function $E_1(1.0, \alpha')$. The straight line corresponds to the exact value $E(1.0)$.

Fig. 2. The function $E^{(1)}(1.0, \alpha')/E^{(0)}(1.0, \alpha')$.

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Tables

Table 1. The exact bound energy $E(\alpha)$ and the results of the asymptotic expansion up to the n-th order $\tilde{E}_n(\alpha)$ $(n = 0,\ 1,\ 2,\ 3)$.

Table 1.

α	$E(\alpha)$	$\tilde{E}_0(\alpha)$	$\tilde{E}_1(\alpha)$	$\tilde{E}_2(\alpha)$	$\tilde{E}_3(\alpha)$
0.1	0.2101	0.2500	0.2074	0.2105	0.2104
0.5	2.426	6.250	0.9292	2.898	2.284
1.0	2.144	25.00	-17.57	13.94	-5.721

Table 2. The exact bound energy $E(\alpha)$, the result of the optimized expansion up to the first order $E_1(\alpha, \alpha_1^{PMS})$ and the results of the odinary perturbation theory up to the n-th order $E_n(\alpha, \alpha)$ $(n = 0,\ 1)$.

Table 2.

α	$E(\alpha)$	$E_1(\alpha, \alpha_1^{PMS})$	$E_0(\alpha)$	$E_1(\alpha, \alpha)$
0.1	0.2101	0.2104	0.2430	0.2092
0.5	2.426	2.424	5.531	1.915
1.0	2.144	2.116	20.13	-4.200

Table 3.The exact bound energy $E(\alpha)$ and various $[i, j]$ Padé approximants $E^{[i,j]}(\alpha)$ with $i + j \leq 3$.

Table 3.

α	$E(\alpha)$	$E^{[1,1]}(\alpha)$	$E^{[0,2]}(\alpha)$	$E^{[2,1]}(\alpha)$	$E^{[1,2]}(\alpha)$	$E^{[0,3]}(\alpha)$
0.1	0.2101	0.2104	0.1874	0.2104	0.2104	0.2104
0.5	2.426	2.366	2.340	2.430	2.424	2.562
1.0	2.144	0.5388	5.759	1.833	1.600	4.331

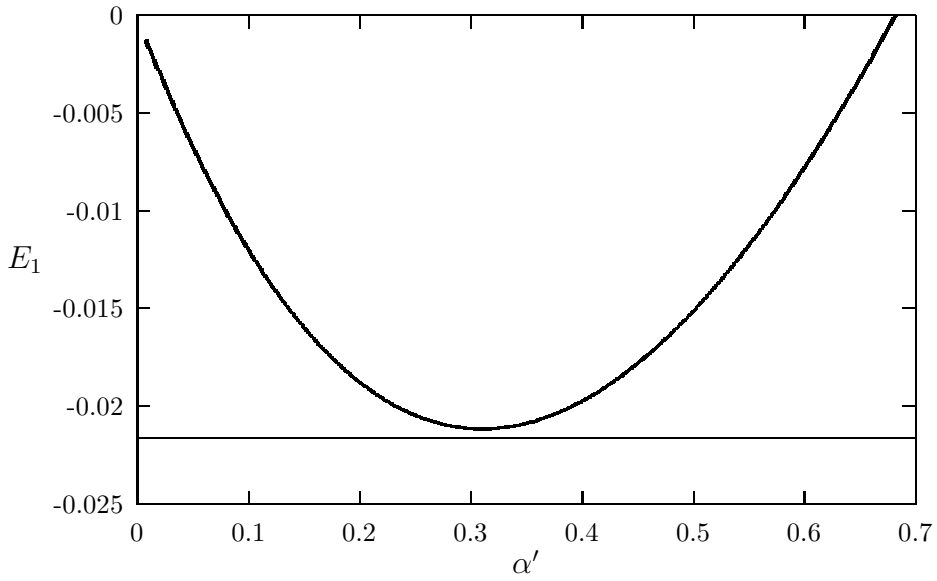

Fig. 1

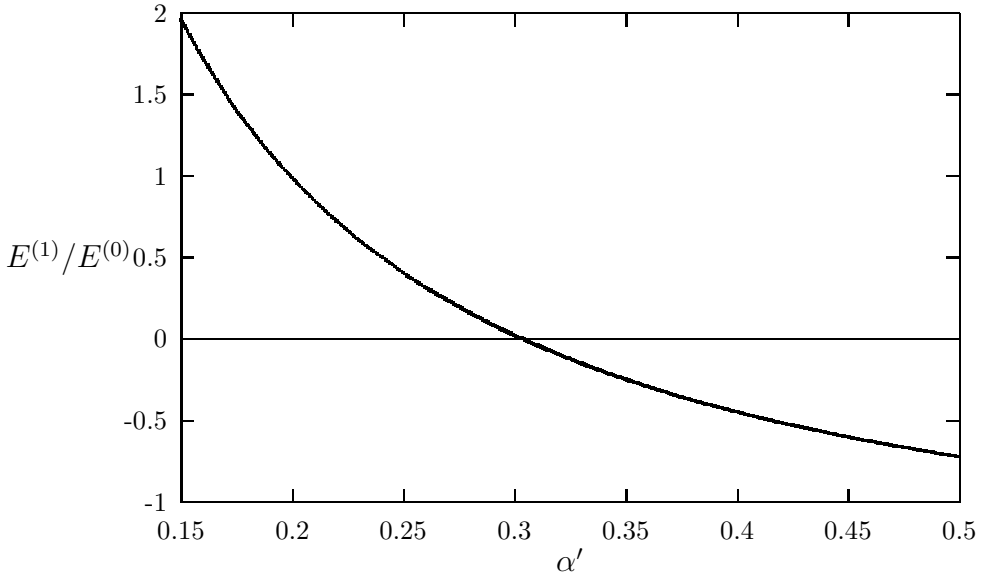

Fig. 2